CLAIMS

1. A method for determining molecular crystal structures from powder diffraction data comprising the steps of: generating a reduced representation of the powder diffraction pattern in dependence on a predetermined unit cell and space group of the molecule under examination in which the total quantity of diffraction data is significantly reduced whilst maintaining the characteristics of the diffraction data that are representative of the crystal structure under examination; determining a set of variables for describing trial molecular structures, derived from predetermined internal co-ordinates and said space group; assigning values to said variables thereby creating a population of trial structures each defined by a unique set of values for said variables; calculating a fitness for each trial structure with respect to the reduced representation of the powder diffraction pattern; determining whether any one of the calculated fitnesses is less than or equal to a predetermined threshold; where none of the calculated fitnesses is less than or equal to the threshold value, selecting at least one survivor from the population of trial structures, altering the values of the variables of at least one of the survivors in accordance with one or more predetermined rules, calculating the fitnesses of the new trial structures; and repeating the steps of selecting survivors, altering the values of the variables and calculating the fitnesses of the new trial structures until at least one of the calculated fitnesses is less than or equal to the threshold value, and where at least one of the calculated fitnesses is less than or equal to the threshold, outputting at least one trial molecular crystal structure represented by the successful sets of values.

2. A method as claimed in claim 1, wherein the reduced representation includes single values representative of the intensity of each

reflection in the powder diffraction data and one or more factors representative of the extent to which adjacent reflections overlap.

3. The method as claimed in claim 2, wherein the reduced representation consists of a structure factor intensity listing and associated covariance matrix.

4. The method as claimed in either of claims 2 or 3, wherein the total data in the reduced representation is reduced by a factor substantially equal to the number of data points in the original powder diffraction data divided by the number Bragg reflections in the measured data range.

5. The method as claimed in either of claims 3 or 4, wherein the fitness χ^2 of each of the trial structures is determined using the following function:

$$\chi^2 = \Sigma_h \Sigma_k \{ (I_h - c|F_h|^2) (V^{-1})_{hk} (I_k - c|F_k|^2) \}$$

where:

$I_{h,k}$ = extracted intensity

V_{hk} = covariance matrix

c = a scale factor

$F_{h,k}$ = calculated structure factor from trial structure

6. The method as claimed in any one of the preceding claims, wherein the set of variables consists of three co-ordinates representative of the location of the molecule within the unit cell and three independent co-ordinates representative of the orientation of the molecule within the unit cell.

7. The method as claimed in claim 6, wherein the set of variables

includes one or more co-ordinates representative of variable torsion angles, bond angles or bond lengths.

8. The method as claimed in any one of the preceding claims including the step of determining the unit cell and space group for the molecule under examination.

9. The method as claimed in any one of the preceding claims including the step of determining the set of internal co-ordinates.

10. The method as claimed in any one of the preceding claims, further including the step of monitoring the number of iterations in which new trial structures are generated and halting the method and outputting the trial crystal structure with the best calculated fitness after completion of a predetermined number of iterations.

11. The method as claimed in any one of the preceding claims, wherein the selection of survivors and the alteration of the values of the variables is based on a simulated annealing procedure.

12. Apparatus for determining molecular crystal structures comprising a structure factor analyser for generating from experimental powder diffraction data for the molecule under examination a reduced representation of the powder diffraction pattern based on a predetermined unit cell and space group in which the total quantity of diffraction data is significantly reduced whilst the characteristics of the diffraction data representative of the crystal structure under examination are maintained; a controller for determining a set of variables for describing trial molecular structures, derived from predetermined internal co-ordinates and said space group; a searching processor for creating a population of trial structures each defined by a unique set of values for said variables said searching

processor including a fitness analyser for calculating a fitness for each trial structure with respect to the reduced representation of the powder diffraction pattern, a thresholding device for determining whether any one of the calculated fitnesses is less than or equal to a predetermined threshold, a survivor selector for selecting at least one survivor from the population of trial structures, a variable adjustment device for altering the values of the variables of at least one of the survivors and output means for outputting the one or more trial molecular crystal structures having calculated fitnesses less than or equal to the threshold value.

13. Apparatus as claimed in claim 12, wherein the reduced representation includes single values representative of the intensity of each reflection in the powder diffraction data and one or more factors representative of the extent to which adjacent reflections overlap.

14. Apparatus as claimed in claim 13, wherein the structure factor analyser generates a reduced representation consists of a structure factor intensity listing and associated covariance matrix.

15. The method as claimed in either of claims 13 or 14, wherein the total data in the reduced representation is reduced by a factor substantially equal to the number of data points in the original powder diffraction data divided by the number Bragg reflections in the measured data range.

16. Apparatus as claimed in either of claims 14 or 15, wherein the fitness analyser determines the fitness χ^2 of each of the trial structures using the following function:

$$\chi^2 = \Sigma_h \Sigma_k \{ (I_h - c|F_h|^2) (V^{-1})_{hk} (I_k - c|F_k|^2) \}$$

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where:

$I_{h,k}$ = extracted intensity from the structure factor analyser

V_{hk} = covariance matrix from the structure factor analyser

c = a scale factor

$F_{h,k}$ = calculated structure factor from trial structure

17. Apparatus as claimed in any one of claims 12 to 16, wherein controller determines a set of variables consists of three co-ordinates representative of the location of the molecule within the unit cell and three independent co-ordinates representative of the orientation of the molecule within the unit.

18. Apparatus as claimed in any one of claims 12 to 17, wherein the structure factor analyser additionally determines the unit cell and space group for the molecule under examination.

19. Apparatus as claimed in any one of claims 12 to 18 including a co-ordinate generator for determining the set of internal co-ordinates.

20. Apparatus as claimed in any one of claims 12 to 19, further including a counter for monitoring the number of iterations of new trial structures.